



Formula: C₁₁H₁₄N₂

MW: 174.25

CAS: 87-52-5

TNP NUMBER: TNP00029

MDL NUMBER: MFCD00005629

IUPAC: (indol-3-ylmethyl)dimethylamine

Smiles: c1ccc2[nH]cc(c2c1)CN(C)C

ACCEPTORS: 0

DONORS: 1

ROTATION BONDS: 1

N+O: 2

Chiral Centers: 0

LogP: 2.54

LogS: -3.6

LIPINSKI: 4

Monograph Number: 0004548

Title: Gramine

CAS Registry Number: 87-52-5

CAS Name: N,N-Dimethyl-1H-indole-3-methanamine

Additional Names: 3-(dimethylaminomethyl)indole

Trademarks: Donaxine

Molecular Formula: C₁₁H₁₄N₂

Molecular Weight: 174.24.

Percent Composition: C 75.83%, H 8.10%, N 16.08%

Literature References: In chlorophyll-deficient mutants of barley: Euler et al., *Z. Physiol. Chem.* 217, 23 (1933). In the Asiatic reed *Arundo donax* L., Gramineae: Orechoff, Norkina, *Ber.* 68, 436 (1935). From *Acer saccharinum* L. (the Silver Maple) and *A. rubrum* L., Aceraceae: Pachter et al., *J. Org. Chem.* 24, 1285 (1959); Pachter, *J. Am. Pharm. Assoc. Sci. Ed.* 48, 670 (1959). Synthesis: K